

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
29 September 2005 (29.09.2005)

PCT

(10) International Publication Number
WO 2005/091178 A2

(51) International Patent Classification⁷: **G06F 17/50**

(72) Inventor; and

(21) International Application Number:
PCT/EP2005/050778

(75) Inventor/Applicant (for US only): **NEUMANN, Marcus, A.** [DE/FR]; 30bis, rue du Vieil Abreuvoir, F-78100 St-Germain-en-Laye (FR).

(22) International Filing Date: 24 February 2005 (24.02.2005)

(74) Agent: **BETTEN & RESCH**; Theatinerstr. 8, 80333 Munich (DE).

(25) Filing Language: English

(26) Publication Language: English

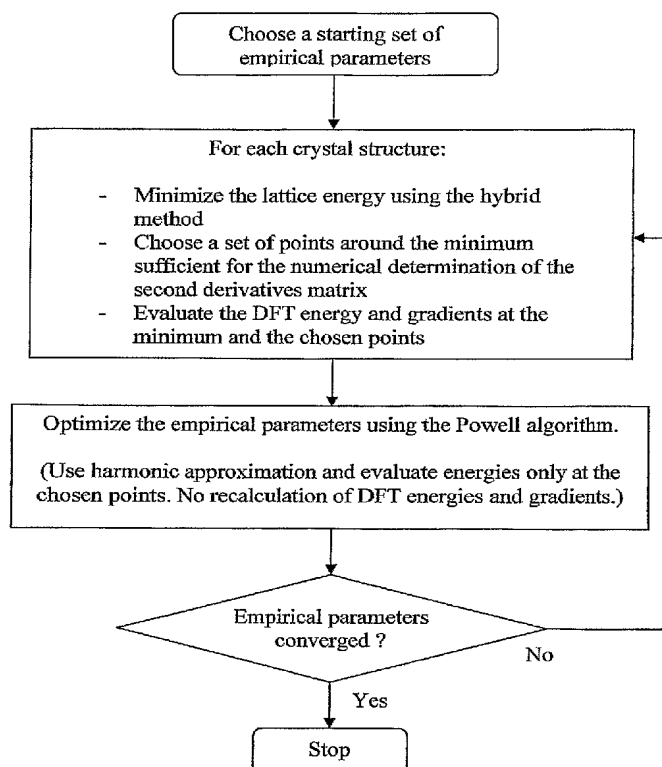
(30) Priority Data:
04290701.4 15 March 2004 (15.03.2004) EP

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(71) Applicant (for all designated States except US):
AVANT-GARDE MATERIALS SIMULATION SARL [FR/FR]; 30bis, rue du Vieil Abreuvoir, F-78100 St-Germain-en-Laye (FR).

[Continued on next page]

(54) Title: ACCURATE ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS



(57) Abstract: The invention refers to a method for the accurate determination of van der Waals parameters for high-precision determination of crystal structures and/or energies, comprising the steps of: numerically simulating at least one crystal structure based on density functional theory (DFT) calculations combined with a potential energy term representing van der Waals interactions; providing reference data containing accurate information about said at least one crystal structure; defining a deviation function (F) quantifying a deviation between said reference data and said at least one simulated crystal structure; fitting at least one parameter of said van der Waals potential term in such a way as to minimize said deviation function (F); and obtaining the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate determination of crystal structures and/or energies based on such a parameter determination as well as the general application of such a hybrid method to the energy ranking of polymorphic crystal structures.



(84) **Designated States** (*unless otherwise indicated, for every kind of regional protection available*): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— *without international search report and to be republished upon receipt of that report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.